

# $\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$

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Key indicators: single-crystal X-ray study;  $T = 293\text{ K}$ ; mean  $\sigma(\text{Co}-\text{O}) = 0.007\text{ \AA}$ ;  $R$  factor = 0.025;  $wR$  factor = 0.056; data-to-parameter ratio = 27.9.

$\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$ , hexalead(II) nonacobalt(II) pentatellurate(VI), is isotypic with its nickel(II) analogue. The asymmetric unit contains two Pb atoms (site symmetries  $\cdot 2$ ,  $\cdot 2$ ), four Co atoms ( $\cdot 2$ ,  $\cdot 2$ ,  $3$ ,  $3$ ), two Te atoms ( $\cdot 2$ ,  $3$ ) and six O atoms (all in general positions), with the Te and Co sites in octahedral coordination environments. The crystal structure can be subdivided into two types of layers parallel to (001). The first layer at  $z \simeq 0.25$  is made up of edge-sharing  $[\text{CoO}_6]$  and  $[\text{TeO}_6]$  octahedra, with 1/6 of the octahedral holes not occupied. The second layer, situated at  $z \simeq 0$ , consist of an alternating arrangement of  $\text{Pb}^{\text{II}}$  atoms and of double octahedra that are made up from face-sharing  $[\text{CoO}_6]$  and  $[\text{TeO}_6]$  octahedra. The two types of layers are linked together through corner-sharing of  $[\text{CoO}_6]$  and  $[\text{TeO}_6]$  octahedra. The  $\text{Pb}^{\text{II}}$  atoms are situated in the cavities of the framework and are stereochemically active with one-sided [4]- and [6]-coordinations, respectively.

## Related literature

For the isotypic nickel analogue, see: Wedel *et al.* (1998). Reviews on the crystal chemistry of oxotellurates(VI) and of the geometry of  $[\text{Co}^{\text{II}}\text{O}_6]$  polyhedra are given by Levason (1997) and Wildner (1992), respectively. For  $\text{Pb}_5\text{TeO}_8$ , see: Artner & Weil (2012). For the bond-valence method, see: Brown (2002).

## Experimental

### Crystal data

$\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$   
 $M_r = 2891.51$   
Hexagonal,  $P6_322$   
 $a = 10.3915(1)\text{ \AA}$   
 $c = 13.6273(2)\text{ \AA}$   
 $V = 1274.37(3)\text{ \AA}^3$   
 $Z = 2$   
Mo  $K\alpha$  radiation

$\mu = 50.89\text{ mm}^{-1}$   
 $T = 293\text{ K}$

$0.07 \times 0.06 \times 0.05\text{ mm}$

### Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: numerical (*HABITUS*; Herrendorf, 1997)  
 $T_{\min} = 0.123$ ,  $T_{\max} = 0.200$   
45686 measured reflections  
2262 independent reflections  
1908 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.068$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.056$   
 $S = 1.09$   
2262 reflections  
81 parameters  
 $\Delta\rho_{\max} = 2.96\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -2.59\text{ e \AA}^{-3}$   
Absolute structure: Flack (1983),  
882 Friedel pairs  
Flack parameter: 0.134 (10)

Table 1

Selected bond lengths ( $\text{\AA}$ ).

Te1—O2	1.906 (5)	Co2—O2	2.090 (6)
Te1—O6	1.991 (4)	Co2—O3 <sup>iii</sup>	2.090 (8)
Te2—O5	1.917 (6)	Co2—O1	2.108 (6)
Te2—O3	1.937 (7)	Co3—O3	2.107 (4)
Te2—O1 <sup>i</sup>	1.939 (5)	Co4—O2	2.067 (7)
Co1—O5 <sup>ii</sup>	2.004 (6)	Co4—O1 <sup>iv</sup>	2.071 (4)
Co1—O6	2.262 (5)	Co4—O5 <sup>v</sup>	2.116 (7)

Symmetry codes: (i)  $x - y, x, z + \frac{1}{2}$ ; (ii)  $-x + y, y, -z + \frac{1}{2}$ ; (iii)  $y, x, -z$ ; (iv)  $-x + y, -x + 1, z$ ; (v)  $x - y, -y + 1, -z$ .

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS for Windows* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2208).

## References

- Artner, C. & Weil, M. (2012). *Z. Kristallogr. Suppl.* **32**, 99.  
Brown, I. D. (2002). In *The Chemical Bond in Inorganic Chemistry: The Bond Valence Model*. Oxford University Press.  
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Dowty, E. (2006). *ATOMS*. Shape Software, Kingsport, Tennessee, USA.  
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
Herrendorf, W. (1997). *HABITUS*. University of Giessen, Germany.  
Levason, W. (1997). *Coord. Chem. Rev.* **161**, 33–79.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Wedel, B., Sugiyama, K. & Müller-Buschbaum, H. K. (1998). *Z. Naturforsch. Teil B*, **53**, 527–531.  
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.  
Wildner, M. (1992). *Z. Kristallogr.* **202**, 51–70.

## supplementary materials

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**Pb<sub>6</sub>Co<sub>9</sub>(TeO<sub>6</sub>)<sub>5</sub>****Christine Artner and Matthias Weil****Comment**

Single crystals of the title compound, Pb<sub>6</sub>Co<sub>9</sub>(TeO<sub>6</sub>)<sub>5</sub>, were serendipitously obtained as a minority phase during phase formation studies in the system Pb<sup>II</sup>/Co<sup>II</sup>/Te<sup>VI</sup>/O intended on crystal growth of cubic Pb<sub>2</sub>CoTeO<sub>6</sub>.

The crystal structure of Pb<sub>6</sub>Co<sub>9</sub>(TeO<sub>6</sub>)<sub>5</sub> is isotypic with its nickel analogue (Wedel *et al.*, 1998). The two Te(VI) and the four Co(II) atoms are in slightly distorted octahedral coordination environments with mean bond lengths of  $\overline{d}(\text{Te—O}) = 1.940 \text{ \AA}$  and  $\overline{d}(\text{Co—O}) = 2.105 \text{ \AA}$ , both in good agreement with literature data for oxotellurates (Levason, 1997) and for [CoO<sub>6</sub>] octahedra (Wildner, 1992). The two lead(II) atoms exhibit coordination numbers of four and six. The corresponding Pb—O, Te—O and M—O (*M* = Co, Ni) bond lengths are very similar in the two isotypic structures.

The crystal structure of Pb<sub>6</sub>Co<sub>9</sub>(TeO<sub>6</sub>)<sub>5</sub> can be described in terms of (001) layers *A* at *z* ≈ 0.25 and *B* at *z* ≈ 0 that stack alternately along [100] (Fig. 1). In layer *A* [TeO<sub>6</sub>] and [CoO<sub>6</sub>] octahedra share edges with 1/6 of the octahedral holes at the 2*c* and 2*d* positions, both with site symmetry 3.2, not occupied. The corresponding vacancies, denominated as *X1* at the 2*d* position and as *X2* at the 2*c* position, have different sizes. *X1* has a diagonal diameter of 4.1076 (8) Å whereas *X2* is somewhat larger with a diagonal diameter of 4.3258 (8) Å. This difference might be correlated with the size of the surrounding octahedra. Whereas the smaller *X1* vacancy is encircled by a ring of six [CoO<sub>6</sub>] octahedra, the larger *X2* is encircled by a ring of three [CoO<sub>6</sub>] and three slightly smaller [TeO<sub>6</sub>] octahedra (Fig. 2). Layer *B* consists of double octahedra that are made up from face-sharing [CoO<sub>6</sub>] and [TeO<sub>6</sub>] octahedra, and by surrounding lead(II) atoms (Fig. 3). Adjacent *A* and *B* layers are linked together above and below the *X1* and *X2* vacancies through corner-sharing of [CoO<sub>6</sub>] and [TeO<sub>6</sub>] octahedra.

The resulting [Co<sub>9</sub>Te<sub>5</sub>O<sub>30</sub>]<sup>12-</sup> framework anion leaves space for the stereochemically active lead(II) cations. The oxygen coordination of the two Pb<sup>2+</sup> cations is one-sided, with a [4]-coordination for Pb1 and a [6]-coordination for Pb2, if only Pb—O distances less than 2.75 Å are taken into account. The two cations share a common edge (O6—O6') with the lone pair electrons *E* pointing towards opposite directions. However, a bond valence calculation (Brown, 2002) shows a significant contribution of the four additional Pb—O distances for each of the two Pb atoms if interactions up to 3.5 Å are considered. Inclusion of these bonds increases the bond valence sum at Pb1 from 1.61 valence units (vu) to 1.83 vu and at Pb2 from 1.64 to 1.96 vu. The bond valence sum at O3 is also raised from 1.60 to 1.80 vu. Therefore the overall coordination of Pb1 might be described as [4 + 4] and that of Pb2 as [6 + 4] (Fig. 4).

**Experimental**

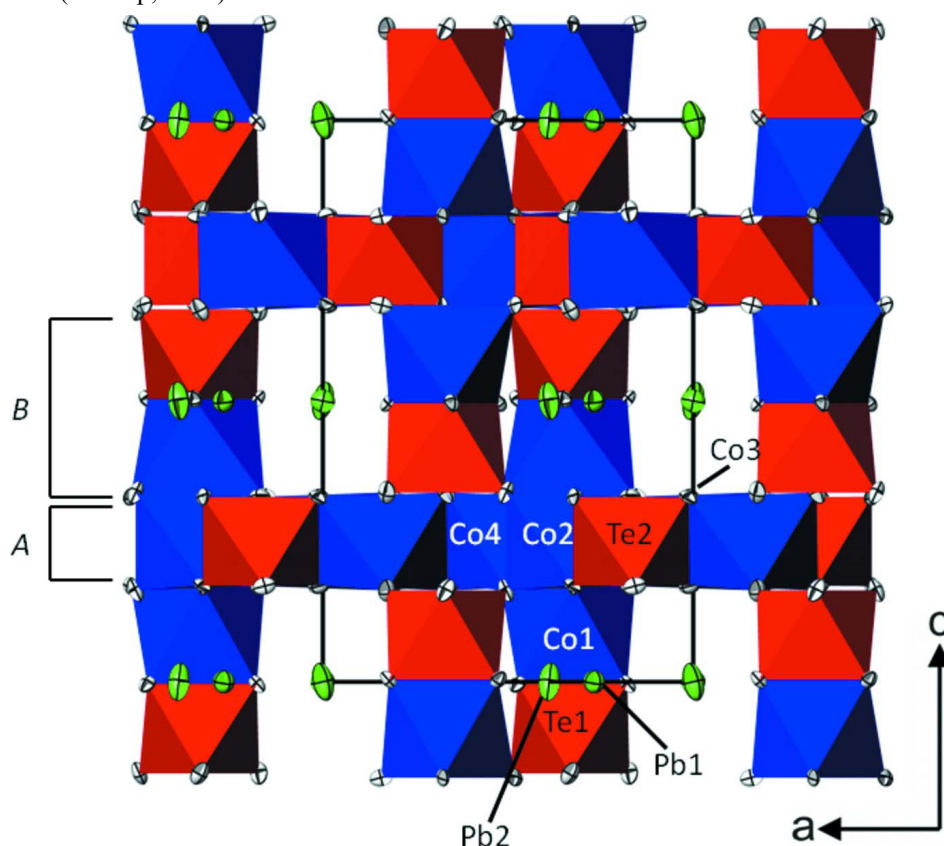
1.281 (5.7 mmol) PbO, 0.216 g (2.9 mmol) CoO and 0.914 g (5.7 mmol) TeO<sub>2</sub> were mixed and thoroughly ground and heated in an alumina crucible under atmospheric conditions during 6 h to 1023 K and held at that temperature for 48 h. Then the furnace was shut-off. Several crystal phases could be identified from the cooled reaction mixture by single-crystal diffraction: Dark blue isometric crystals of Pb<sub>2</sub>CoTeO<sub>6</sub>, dark-red (nearly black) block-like crystals of Pb<sub>5</sub>TeO<sub>8</sub> (Artner & Weil, 2012), colourless crystals of α-Al<sub>2</sub>O<sub>3</sub> and dark red crystals of Pb<sub>6</sub>Co<sub>9</sub>(TeO<sub>6</sub>)<sub>5</sub> with a block-like shape.

## Refinement

The highest remaining electron density was found 1.49 Å from atom Pb1 and the lowest remaining electron density 0.52 Å from atom Pb2. The refined Flack parameter indicates racemic twinning with an approximate ratio of 1:6 for the twin components.

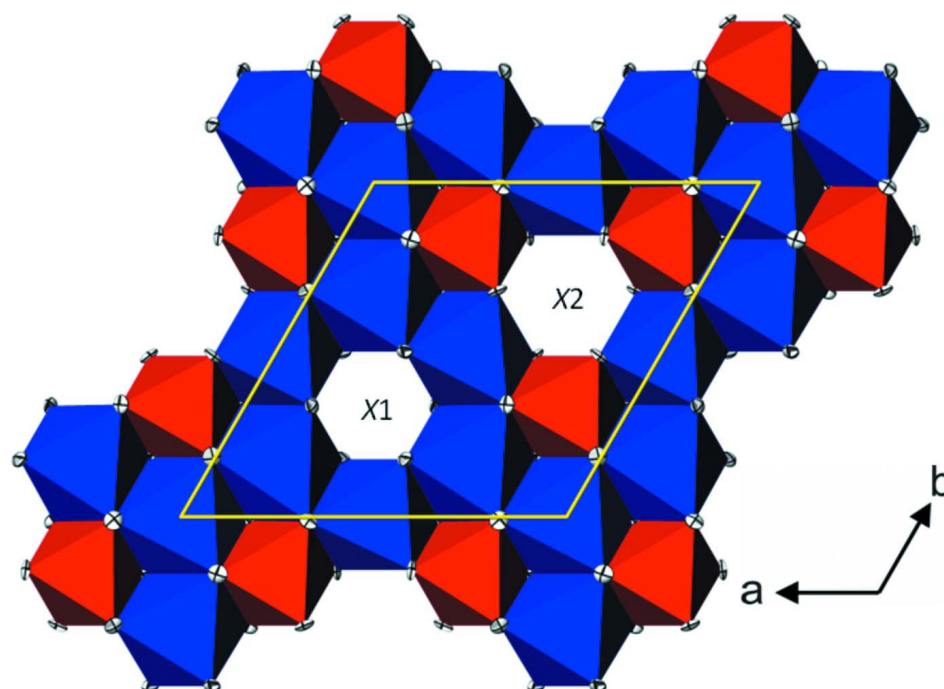
## Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS for Windows* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).



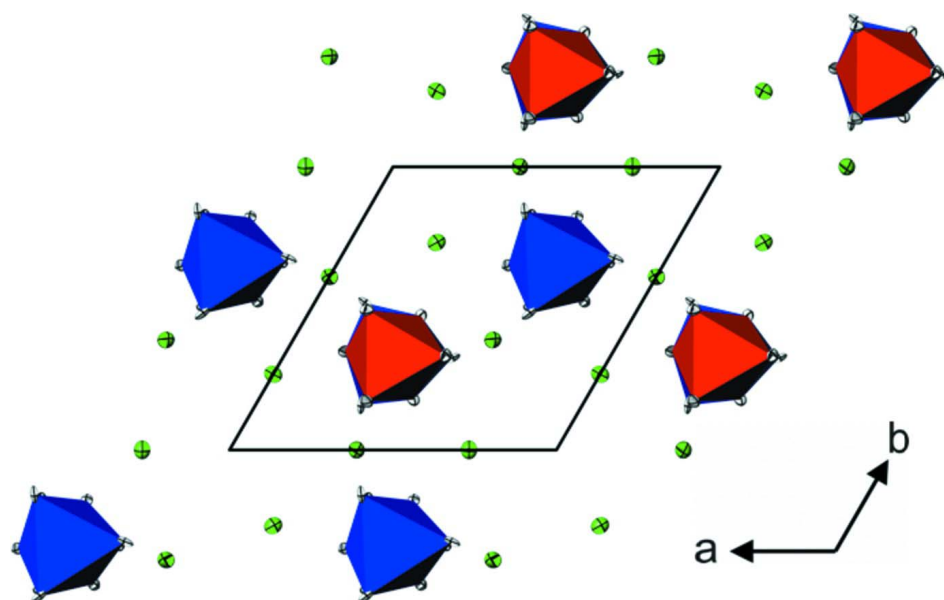
**Figure 1**

The crystal structure of  $\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$  in a projection along  $[010]$ . Displacement ellipsoids are drawn at the 90% probability level. Letters *A* and *B* indicate the two types of layers present in the structure.



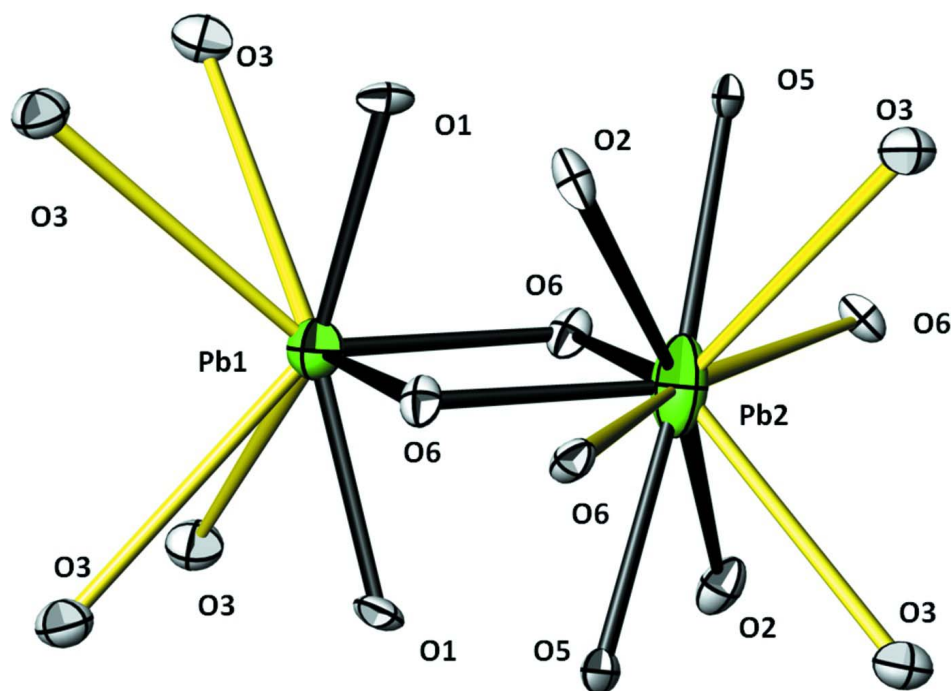
**Figure 2**

Layer *A* (situated approximately at  $z \approx 1/4$ ) in the crystal structure of  $\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$ . Colour code and probability of the displacement parameters as in Fig. 1.



**Figure 3**

Layer *B* (situated approximately at  $z \approx 0$ ) in the crystal structure of  $\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$ . Colour code and probability of the displacement parameters as in Fig. 1.



**Figure 4**

The coordination spheres around the two lead atoms, considering bond lengths up to 3.5 Å; short Pb—O distances < 2.75 Å are given in black, emphasizing the one-sided [4]-coordination for Pb1 and [6]-coordination for Pb2. Longer bonds augmenting the coordination spheres are given in yellow. Probability of the displacement parameters as in Fig. 1.

#### hexalead(II) nonacobalt(II) pentatellurate(VI)

##### Crystal data

$\text{Pb}_6\text{Co}_9(\text{TeO}_6)_5$   
 $M_r = 2891.51$   
 Hexagonal,  $P6_322$   
 Hall symbol:  $P\ 6c\ 2c$   
 $a = 10.3915\ (1)\ \text{\AA}$   
 $c = 13.6273\ (2)\ \text{\AA}$   
 $V = 1274.37\ (3)\ \text{\AA}^3$   
 $Z = 2$   
 $F(000) = 2470$

$D_x = 7.535\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 6739 reflections  
 $\theta = 2.8\text{--}36.8^\circ$   
 $\mu = 50.89\ \text{mm}^{-1}$   
 $T = 293\ \text{K}$   
 Parallelepiped, dark red  
 $0.07 \times 0.06 \times 0.05\ \text{mm}$

##### Data collection

Bruker APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: numerical  
 (*HABITUS*; Herrendorf, 1997)  
 $T_{\min} = 0.123$ ,  $T_{\max} = 0.200$

45686 measured reflections  
 2262 independent reflections  
 1908 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.068$   
 $\theta_{\max} = 37.6^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -16 \rightarrow 17$   
 $k = -17 \rightarrow 17$   
 $l = -22 \rightarrow 23$

# Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.025$ 
 $wR(F^2) = 0.056$ 
 $S = 1.09$ 

2262 reflections

81 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

 $w = 1/[\sigma^2(F_o^2) + (0.0244P)^2]$ 

where  $P = (F_o^2 + 2F_c^2)/3$ 
 $(\Delta/\sigma)_{\max} < 0.001$ 
 $\Delta\rho_{\max} = 2.96 \text{ e } \text{\AA}^{-3}$ 
 $\Delta\rho_{\min} = -2.59 \text{ e } \text{\AA}^{-3}$ 

Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.00019 (3)

Absolute structure: Flack (1983), 882 Friedel  
pairs

Flack parameter: 0.134 (10)

# Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

# Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb1	0.26736 (3)	0.26736 (3)	0.0000	0.01216 (6)
Pb2	0.38848 (3)	1.0000	0.0000	0.01881 (8)
Te1	0.3333	0.6667	−0.09611 (4)	0.00407 (10)
Te2	0.16730 (4)	0.33460 (9)	0.2500	0.00433 (8)
Co1	0.3333	0.6667	0.11832 (9)	0.0066 (2)
Co2	0.16885 (10)	0.3377 (2)	−0.2500	0.00664 (18)
Co3	0.0000	0.0000	0.2500	0.0087 (3)
Co4	0.00992 (19)	0.50496 (10)	−0.2500	0.00566 (18)
O1	0.3366 (5)	0.3241 (5)	−0.1717 (3)	0.0077 (8)
O2	0.1726 (7)	0.5050 (6)	−0.1628 (3)	0.0083 (10)
O3	0.1702 (7)	0.1801 (6)	0.3277 (3)	0.0105 (9)
O5	0.3239 (8)	0.4818 (6)	0.3295 (3)	0.0076 (10)
O6	0.3481 (4)	0.5265 (4)	−0.0034 (4)	0.0069 (6)

# Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pb1	0.01117 (9)	0.01117 (9)	0.01243 (12)	0.00429 (9)	0.00014 (9)	−0.00014 (9)
Pb2	0.01104 (9)	0.01201 (13)	0.03372 (18)	0.00601 (7)	−0.00268 (13)	−0.0054 (3)
Te1	0.00414 (14)	0.00414 (14)	0.0039 (2)	0.00207 (7)	0.000	0.000
Te2	0.00362 (13)	0.00380 (19)	0.00564 (18)	0.00190 (10)	0.0002 (4)	0.000
Co1	0.0066 (3)	0.0066 (3)	0.0066 (5)	0.00332 (16)	0.000	0.000
Co2	0.0057 (3)	0.0069 (5)	0.0077 (4)	0.0035 (2)	0.0006 (10)	0.000
Co3	0.0061 (4)	0.0061 (4)	0.0140 (7)	0.00305 (19)	0.000	0.000

Co4	0.0031 (5)	0.0045 (3)	0.0089 (4)	0.0015 (2)	0.000	−0.0002 (3)
O1	0.011 (2)	0.008 (2)	0.0048 (15)	0.0055 (14)	0.0003 (13)	−0.0022 (13)
O2	0.007 (2)	0.006 (2)	0.012 (2)	0.0022 (17)	−0.0001 (16)	−0.0034 (15)
O3	0.011 (2)	0.012 (2)	0.0077 (16)	0.0059 (15)	0.0000 (15)	0.0011 (15)
O5	0.004 (2)	0.006 (2)	0.0072 (18)	−0.0011 (18)	−0.0005 (18)	0.0009 (15)
O6	0.0058 (14)	0.0070 (14)	0.0075 (15)	0.0029 (11)	−0.001 (2)	0.002 (2)

*Geometric parameters (Å, °)*

Pb1—O6 <sup>i</sup>	2.387 (4)	Te2—O3 <sup>iii</sup>	1.937 (7)
Pb1—O6	2.387 (4)	Te2—O3	1.937 (7)
Pb1—O1 <sup>i</sup>	2.432 (4)	Te2—O1 <sup>xii</sup>	1.939 (5)
Pb1—O1	2.432 (4)	Te2—O1 <sup>i</sup>	1.939 (5)
Pb1—O3 <sup>ii</sup>	3.327 (7)	Co1—O5 <sup>x</sup>	2.004 (6)
Pb1—O3 <sup>iii</sup>	3.327 (7)	Co1—O5 <sup>iii</sup>	2.004 (6)
Pb1—O3 <sup>iv</sup>	3.453 (7)	Co1—O5 <sup>xiii</sup>	2.004 (6)
Pb1—O3 <sup>v</sup>	3.453 (7)	Co1—O6 <sup>vi</sup>	2.262 (5)
Pb1—Pb2 <sup>vi</sup>	3.5764 (4)	Co1—O6 <sup>vii</sup>	2.262 (5)
Pb1—Pb2 <sup>vii</sup>	3.5777 (2)	Co1—O6	2.262 (5)
Pb2—O6 <sup>viii</sup>	2.420 (3)	Co2—O2 <sup>xiv</sup>	2.090 (6)
Pb2—O6 <sup>vii</sup>	2.420 (3)	Co2—O2	2.090 (6)
Pb2—O2 <sup>ix</sup>	2.726 (5)	Co2—O3 <sup>i</sup>	2.090 (8)
Pb2—O2 <sup>vi</sup>	2.726 (5)	Co2—O3 <sup>iv</sup>	2.090 (8)
Pb2—O5 <sup>x</sup>	2.727 (5)	Co2—O1	2.108 (6)
Pb2—O5 <sup>xi</sup>	2.727 (5)	Co2—O1 <sup>xiv</sup>	2.108 (6)
Pb2—O6 <sup>vi</sup>	3.155 (3)	Co3—O3 <sup>xv</sup>	2.107 (4)
Pb2—O6 <sup>ix</sup>	3.155 (3)	Co3—O3	2.107 (4)
Pb2—O3 <sup>xi</sup>	3.230 (4)	Co3—O3 <sup>xvi</sup>	2.107 (4)
Pb2—O3 <sup>x</sup>	3.230 (4)	Co3—O3 <sup>xvii</sup>	2.107 (4)
Te1—O2 <sup>vi</sup>	1.906 (5)	Co3—O3 <sup>iii</sup>	2.107 (4)
Te1—O2	1.906 (5)	Co3—O3 <sup>v</sup>	2.107 (4)
Te1—O2 <sup>vii</sup>	1.906 (5)	Co4—O2	2.067 (7)
Te1—O6 <sup>vi</sup>	1.991 (4)	Co4—O2 <sup>xviii</sup>	2.067 (7)
Te1—O6 <sup>vii</sup>	1.991 (4)	Co4—O1 <sup>vi</sup>	2.071 (4)
Te1—O6	1.991 (4)	Co4—O1 <sup>xiv</sup>	2.071 (4)
Te2—O5	1.917 (6)	Co4—O5 <sup>xix</sup>	2.116 (7)
Te2—O5 <sup>iii</sup>	1.917 (6)	Co4—O5 <sup>iv</sup>	2.116 (7)
O6 <sup>i</sup> —Pb1—O6	84.58 (16)	O5 <sup>iii</sup> —Te2—O1 <sup>xii</sup>	85.9 (2)
O6 <sup>i</sup> —Pb1—O1 <sup>i</sup>	79.26 (18)	O3 <sup>iii</sup> —Te2—O1 <sup>xii</sup>	87.0 (2)
O6—Pb1—O1 <sup>i</sup>	77.79 (18)	O3—Te2—O1 <sup>xii</sup>	93.7 (2)
O6 <sup>i</sup> —Pb1—O1	77.79 (18)	O5—Te2—O1 <sup>i</sup>	85.9 (2)
O6—Pb1—O1	79.26 (18)	O5 <sup>iii</sup> —Te2—O1 <sup>i</sup>	93.3 (2)
O1 <sup>i</sup> —Pb1—O1	148.79 (19)	O3 <sup>iii</sup> —Te2—O1 <sup>i</sup>	93.7 (2)
O6 <sup>i</sup> —Pb1—O3 <sup>ii</sup>	95.87 (13)	O3—Te2—O1 <sup>i</sup>	87.0 (2)
O6—Pb1—O3 <sup>ii</sup>	133.98 (17)	O1 <sup>xii</sup> —Te2—O1 <sup>i</sup>	179.0 (3)
O1 <sup>i</sup> —Pb1—O3 <sup>ii</sup>	147.68 (15)	O5 <sup>x</sup> —Co1—O5 <sup>iii</sup>	108.14 (14)
O1—Pb1—O3 <sup>ii</sup>	56.26 (15)	O5 <sup>x</sup> —Co1—O5 <sup>xiii</sup>	108.14 (14)
O6 <sup>i</sup> —Pb1—O3 <sup>iii</sup>	133.98 (17)	O5 <sup>iii</sup> —Co1—O5 <sup>xiii</sup>	108.14 (14)
O6—Pb1—O3 <sup>iii</sup>	95.87 (13)	O5 <sup>x</sup> —Co1—O6 <sup>vi</sup>	87.99 (18)

O1 <sup>i</sup> —Pb1—O3 <sup>iii</sup>	56.26 (15)	O5 <sup>iii</sup> —Co1—O6 <sup>vi</sup>	85.39 (19)
O1—Pb1—O3 <sup>iii</sup>	147.68 (15)	O5 <sup>xiii</sup> —Co1—O6 <sup>vi</sup>	153.55 (18)
O3 <sup>ii</sup> —Pb1—O3 <sup>iii</sup>	114.8 (2)	O5 <sup>x</sup> —Co1—O6 <sup>vii</sup>	85.39 (19)
O6 <sup>i</sup> —Pb1—O3 <sup>iv</sup>	138.20 (17)	O5 <sup>iii</sup> —Co1—O6 <sup>vii</sup>	153.55 (18)
O6—Pb1—O3 <sup>iv</sup>	95.05 (13)	O5 <sup>xiii</sup> —Co1—O6 <sup>vii</sup>	87.99 (18)
O1 <sup>i</sup> —Pb1—O3 <sup>iv</sup>	141.63 (15)	O6 <sup>vi</sup> —Co1—O6 <sup>vii</sup>	72.17 (17)
O1—Pb1—O3 <sup>iv</sup>	61.26 (14)	O5 <sup>x</sup> —Co1—O6	153.55 (18)
O3 <sup>ii</sup> —Pb1—O3 <sup>iv</sup>	55.44 (13)	O5 <sup>iii</sup> —Co1—O6	87.99 (18)
O3 <sup>iii</sup> —Pb1—O3 <sup>iv</sup>	87.73 (10)	O5 <sup>xiii</sup> —Co1—O6	85.39 (18)
O6 <sup>i</sup> —Pb1—O3 <sup>v</sup>	95.05 (13)	O6 <sup>vi</sup> —Co1—O6	72.17 (17)
O6—Pb1—O3 <sup>v</sup>	138.20 (17)	O6 <sup>vii</sup> —Co1—O6	72.17 (17)
O1 <sup>i</sup> —Pb1—O3 <sup>v</sup>	61.26 (14)	O2 <sup>xiv</sup> —Co2—O2	87.8 (3)
O1—Pb1—O3 <sup>v</sup>	141.63 (15)	O2 <sup>xiv</sup> —Co2—O3 <sup>i</sup>	92.52 (17)
O3 <sup>ii</sup> —Pb1—O3 <sup>v</sup>	87.73 (10)	O2—Co2—O3 <sup>i</sup>	174.4 (3)
O3 <sup>iii</sup> —Pb1—O3 <sup>v</sup>	55.44 (13)	O2 <sup>xiv</sup> —Co2—O3 <sup>iv</sup>	174.4 (3)
O3 <sup>iv</sup> —Pb1—O3 <sup>v</sup>	111.4 (2)	O2—Co2—O3 <sup>iv</sup>	92.52 (17)
O6 <sup>viii</sup> —Pb2—O6 <sup>vii</sup>	83.17 (17)	O3 <sup>i</sup> —Co2—O3 <sup>iv</sup>	87.7 (2)
O6 <sup>viii</sup> —Pb2—O2 <sup>ix</sup>	61.34 (16)	O2 <sup>xiv</sup> —Co2—O1	89.3 (2)
O6 <sup>vii</sup> —Pb2—O2 <sup>ix</sup>	107.91 (19)	O2—Co2—O1	95.5 (2)
O6 <sup>viii</sup> —Pb2—O2 <sup>vi</sup>	107.91 (19)	O3 <sup>i</sup> —Co2—O1	78.9 (2)
O6 <sup>vii</sup> —Pb2—O2 <sup>vi</sup>	61.34 (16)	O3 <sup>iv</sup> —Co2—O1	96.2 (2)
O2 <sup>ix</sup> —Pb2—O2 <sup>vi</sup>	166.8 (3)	O2 <sup>xiv</sup> —Co2—O1 <sup>xiv</sup>	95.5 (2)
O6 <sup>viii</sup> —Pb2—O5 <sup>x</sup>	106.77 (19)	O2—Co2—O1 <sup>xiv</sup>	89.3 (2)
O6 <sup>vii</sup> —Pb2—O5 <sup>x</sup>	68.25 (16)	O3 <sup>i</sup> —Co2—O1 <sup>xiv</sup>	96.2 (2)
O2 <sup>ix</sup> —Pb2—O5 <sup>x</sup>	66.27 (12)	O3 <sup>iv</sup> —Co2—O1 <sup>xiv</sup>	78.9 (2)
O2 <sup>vi</sup> —Pb2—O5 <sup>x</sup>	112.94 (13)	O1—Co2—O1 <sup>xiv</sup>	173.3 (3)
O6 <sup>viii</sup> —Pb2—O5 <sup>xi</sup>	68.25 (16)	O3 <sup>xv</sup> —Co3—O3	175.2 (5)
O6 <sup>vii</sup> —Pb2—O5 <sup>xi</sup>	106.77 (19)	O3 <sup>xv</sup> —Co3—O3 <sup>xvi</sup>	79.5 (4)
O2 <sup>ix</sup> —Pb2—O5 <sup>xi</sup>	112.94 (13)	O3—Co3—O3 <sup>xvi</sup>	96.96 (14)
O2 <sup>vi</sup> —Pb2—O5 <sup>xi</sup>	66.27 (12)	O3 <sup>xv</sup> —Co3—O3 <sup>xvii</sup>	86.8 (4)
O5 <sup>x</sup> —Pb2—O5 <sup>xi</sup>	173.7 (3)	O3—Co3—O3 <sup>xvii</sup>	96.96 (14)
O6 <sup>viii</sup> —Pb2—O6 <sup>vi</sup>	138.39 (2)	O3 <sup>xvi</sup> —Co3—O3 <sup>xvii</sup>	96.96 (14)
O6 <sup>vii</sup> —Pb2—O6 <sup>vi</sup>	55.23 (15)	O3 <sup>xv</sup> —Co3—O3 <sup>iii</sup>	96.96 (14)
O2 <sup>ix</sup> —Pb2—O6 <sup>vi</sup>	126.25 (15)	O3—Co3—O3 <sup>iii</sup>	79.5 (4)
O2 <sup>vi</sup> —Pb2—O6 <sup>vi</sup>	55.67 (17)	O3 <sup>xvi</sup> —Co3—O3 <sup>iii</sup>	86.8 (4)
O5 <sup>x</sup> —Pb2—O6 <sup>vi</sup>	60.10 (16)	O3 <sup>xvii</sup> —Co3—O3 <sup>iii</sup>	175.2 (5)
O5 <sup>xi</sup> —Pb2—O6 <sup>vi</sup>	120.76 (15)	O3 <sup>xv</sup> —Co3—O3 <sup>v</sup>	96.96 (14)
O6 <sup>viii</sup> —Pb2—O6 <sup>ix</sup>	55.23 (15)	O3—Co3—O3 <sup>v</sup>	86.8 (4)
O6 <sup>vii</sup> —Pb2—O6 <sup>ix</sup>	138.39 (2)	O3 <sup>xvi</sup> —Co3—O3 <sup>v</sup>	175.2 (5)
O2 <sup>ix</sup> —Pb2—O6 <sup>ix</sup>	55.67 (17)	O3 <sup>xvii</sup> —Co3—O3 <sup>v</sup>	79.5 (4)
O2 <sup>vi</sup> —Pb2—O6 <sup>ix</sup>	126.25 (15)	O3 <sup>iii</sup> —Co3—O3 <sup>v</sup>	96.96 (14)
O5 <sup>x</sup> —Pb2—O6 <sup>ix</sup>	120.76 (15)	O2—Co4—O2 <sup>xviii</sup>	89.8 (3)
O5 <sup>xi</sup> —Pb2—O6 <sup>ix</sup>	60.10 (16)	O2—Co4—O1 <sup>vi</sup>	96.9 (2)
O6 <sup>vi</sup> —Pb2—O6 <sup>ix</sup>	166.38 (13)	O2 <sup>xviii</sup> —Co4—O1 <sup>vi</sup>	91.0 (2)
O6 <sup>viii</sup> —Pb2—O3 <sup>xi</sup>	120.59 (18)	O2—Co4—O1 <sup>xiv</sup>	91.0 (2)
O6 <sup>vii</sup> —Pb2—O3 <sup>xi</sup>	121.18 (18)	O2 <sup>xviii</sup> —Co4—O1 <sup>xiv</sup>	96.9 (2)
O2 <sup>ix</sup> —Pb2—O3 <sup>xi</sup>	130.9 (2)	O1 <sup>vi</sup> —Co4—O1 <sup>xiv</sup>	168.8 (4)
O2 <sup>vi</sup> —Pb2—O3 <sup>xi</sup>	60.21 (13)	O2—Co4—O5 <sup>xix</sup>	174.7 (3)
O5 <sup>x</sup> —Pb2—O3 <sup>xi</sup>	132.1 (2)	O2 <sup>xviii</sup> —Co4—O5 <sup>xix</sup>	90.92 (16)



O5 <sup>xi</sup> —Pb2—O3 <sup>xi</sup>	53.44 (14)	O1 <sup>vi</sup> —Co4—O5 <sup>xix</sup>	77.8 (2)
O6 <sup>vi</sup> —Pb2—O3 <sup>xi</sup>	86.29 (19)	O1 <sup>xiv</sup> —Co4—O5 <sup>xix</sup>	94.2 (2)
O6 <sup>ix</sup> —Pb2—O3 <sup>xi</sup>	84.37 (18)	O2—Co4—O5 <sup>iv</sup>	90.92 (16)
O6 <sup>viii</sup> —Pb2—O3 <sup>x</sup>	121.18 (18)	O2 <sup>xviii</sup> —Co4—O5 <sup>iv</sup>	174.7 (3)
O6 <sup>vii</sup> —Pb2—O3 <sup>x</sup>	120.59 (18)	O1 <sup>vi</sup> —Co4—O5 <sup>iv</sup>	94.2 (2)
O2 <sup>ix</sup> —Pb2—O3 <sup>x</sup>	60.21 (13)	O1 <sup>xiv</sup> —Co4—O5 <sup>iv</sup>	77.8 (2)
O2 <sup>vi</sup> —Pb2—O3 <sup>x</sup>	130.9 (2)	O5 <sup>xix</sup> —Co4—O5 <sup>iv</sup>	88.9 (3)
O5 <sup>x</sup> —Pb2—O3 <sup>x</sup>	53.44 (14)	Te2 <sup>ii</sup> —O1—Co4 <sup>vii</sup>	98.54 (19)
O5 <sup>xi</sup> —Pb2—O3 <sup>x</sup>	132.1 (2)	Te2 <sup>ii</sup> —O1—Co2	96.67 (17)
O6 <sup>vi</sup> —Pb2—O3 <sup>x</sup>	84.37 (18)	Co4 <sup>vii</sup> —O1—Co2	89.3 (2)
O6 <sup>ix</sup> —Pb2—O3 <sup>x</sup>	86.29 (19)	Te2 <sup>ii</sup> —O1—Pb1	116.6 (2)
O3 <sup>xi</sup> —Pb2—O3 <sup>x</sup>	93.32 (14)	Co4 <sup>vii</sup> —O1—Pb1	136.07 (18)
O2 <sup>vi</sup> —Te1—O2	99.15 (18)	Co2—O1—Pb1	110.4 (2)
O2 <sup>vi</sup> —Te1—O2 <sup>vii</sup>	99.15 (18)	Te1—O2—Co4	129.1 (3)
O2—Te1—O2 <sup>vii</sup>	99.15 (18)	Te1—O2—Co2	130.4 (4)
O2 <sup>vi</sup> —Te1—O6 <sup>vi</sup>	90.7 (2)	Co4—O2—Co2	89.87 (19)
O2—Te1—O6 <sup>vi</sup>	85.2 (2)	Te1—O2—Pb2 <sup>vii</sup>	95.48 (17)
O2 <sup>vii</sup> —Te1—O6 <sup>vi</sup>	168.4 (2)	Co4—O2—Pb2 <sup>vii</sup>	96.4 (2)
O2 <sup>vi</sup> —Te1—O6 <sup>vii</sup>	85.2 (2)	Co2—O2—Pb2 <sup>vii</sup>	111.0 (2)
O2—Te1—O6 <sup>vii</sup>	168.4 (2)	Te2—O3—Co2 <sup>xx</sup>	97.34 (17)
O2 <sup>vii</sup> —Te1—O6 <sup>vii</sup>	90.7 (2)	Te2—O3—Co3	96.2 (2)
O6 <sup>vi</sup> —Te1—O6 <sup>vii</sup>	84.0 (2)	Co2 <sup>xx</sup> —O3—Co3	92.8 (3)
O2 <sup>vi</sup> —Te1—O6	168.4 (2)	Te2—O5—Co1 <sup>xiii</sup>	125.5 (4)
O2—Te1—O6	90.7 (2)	Te2—O5—Co4 <sup>xx</sup>	97.7 (2)
O2 <sup>vii</sup> —Te1—O6	85.2 (2)	Co1 <sup>xiii</sup> —O5—Co4 <sup>xx</sup>	120.3 (3)
O6 <sup>vi</sup> —Te1—O6	84.0 (2)	Te2—O5—Pb2 <sup>xxi</sup>	117.3 (2)
O6 <sup>vii</sup> —Te1—O6	84.0 (2)	Co1 <sup>xiii</sup> —O5—Pb2 <sup>xxi</sup>	97.82 (18)
O5—Te2—O5 <sup>iii</sup>	92.5 (3)	Co4 <sup>xx</sup> —O5—Pb2 <sup>xxi</sup>	95.2 (2)
O5—Te2—O3 <sup>iii</sup>	177.8 (2)	Te1—O6—Co1	86.54 (14)
O5 <sup>iii</sup> —Te2—O3 <sup>iii</sup>	89.6 (2)	Te1—O6—Pb1	136.5 (2)
O5—Te2—O3	89.6 (2)	Co1—O6—Pb1	127.8 (2)
O5 <sup>iii</sup> —Te2—O3	177.8 (2)	Te1—O6—Pb2 <sup>vi</sup>	103.41 (16)
O3 <sup>iii</sup> —Te2—O3	88.2 (2)	Co1—O6—Pb2 <sup>vi</sup>	100.34 (16)
O5—Te2—O1 <sup>xii</sup>	93.3 (2)	Pb1—O6—Pb2 <sup>vi</sup>	96.12 (13)

Symmetry codes: (i)  $y, x, -z$ ; (ii)  $y, -x+y, z-1/2$ ; (iii)  $-x+y, y, -z+1/2$ ; (iv)  $x-y, x, z-1/2$ ; (v)  $x, x-y, -z+1/2$ ; (vi)  $-x+y, -x+1, z$ ; (vii)  $-y+1, x-y+1, z$ ; (viii)  $-x+1, -x+y+1, -z$ ; (ix)  $y, x+1, -z$ ; (x)  $x, x-y+1, -z+1/2$ ; (xi)  $y, -x+y+1, z-1/2$ ; (xii)  $x-y, x, z+1/2$ ; (xiii)  $-y+1, -x+1, -z+1/2$ ; (xiv)  $-x+y, y, -z-1/2$ ; (xv)  $-y, -x, -z+1/2$ ; (xvi)  $-y, x-y, z$ ; (xvii)  $-x+y, -x, z$ ; (xviii)  $x, x-y+1, -z-1/2$ ; (xix)  $x-y, -y+1, -z$ ; (xx)  $y, -x+y, z+1/2$ ; (xxi)  $x-y+1, x, z+1/2$ .